

THE CONTRIBUTION OF TOBACCO CONSTITUENTS TO PHENOL YIELD OF CIGARETTES.

A. W. Spears, J. H. Bell and A. O. Saunders, Research Division, P. Lorillard Company, Greensboro, North Carolina.

ABSTRACT

Phenol has been a reported component of cigarette smoke for many years, but no occurrence in American tobaccos has been reported. Obviously, phenol is formed during the smoking process and differences in phenol yield may be found between tobacco types (Bright and Burley). Pyrolysis studies were carried out at various temperatures in both air and nitrogen with Bright and Burley tobaccos until conditions were found which gave the same ratio of phenol yield as obtained with the respective cigarettes on smoking. Using these conditions, leaf extracts and leaf components were pyrolyzed and phenol yields determined. Both the method and data will be presented. On the basis of the pyrolysis studies, uniformly labeled C<sup>14</sup> glucose was added to tobacco and after preparation of cigarettes and smoking, the incorporation of radioactivity into phenol was determined. Data will be presented. Both the data from pyrolysis studies and the addition of C<sup>14</sup> glucose to cigarettes will be discussed, and the role of carbohydrates as precursors of phenol will be evaluated. The data provide some information with respect to the mechanism of phenol formation and some inferences will be made. In general, it is thought that these techniques provide a means for elucidating smoke precursors, but certain limitations exist which will be indicated in the discussion.

REVIEW BY M. D. EDMONDS

A method was presented for the pyrolysis of individual tobacco constituents and burley and bright tobaccos, and a measurement of phenol was obtained from the pyrolysates.

The pyrolysis apparatus was quite similar to the one used here at the Research Center. The samples were pyrolyzed in both oxygen and nitrogen atmospheres. The trapped samples were collected at dry ice-acetone temperature. The phenol content was measured by the procedure of A. W. Spears, Quantitative Determination of Phenol, Anal. Chem., 35, 320-322 (1963).

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The following data were presented:

Percent Conversion To Phenol

	<u>Air Atm-100 ml/min.</u>	<u>N<sub>2</sub>-100 ml/min.</u>
Glucose	$5.0 \times 10^{-2}$	$7.7 \times 10^{-2}$
Sucrose	$6.7 \times 10^{-2}$	$6.2 \times 10^{-2}$
Starch	$2.2 \times 10^{-3}$	$3.0 \times 10^{-2}$
Cellulose	$2.4 \times 10^{-2}$	$8.0 \times 10^{-3}$
Pectin	$2.6 \times 10^{-2}$	$1.7 \times 10^{-2}$
Rutin	$8.0 \times 10^{-3}$	$4.0 \times 10^{-3}$
Chlorogenic Acid	---	$8.0 \times 10^{-3}$
Flue Cured Tobacco	$5.0 \times 10^{-2}$	$2.9 \times 10^{-2}$
Burley Tobacco	$4.7 \times 10^{-2}$	$2.6 \times 10^{-2}$
Stationary Furnace 1 =	$315^{\circ}\text{C}$	$777^{\circ}\text{C}$
Stationary Furnace 2 =	$320^{\circ}\text{C}$	$562^{\circ}\text{C}$
Mobile Furnace	= $685^{\circ}\text{C}$	$685^{\circ}\text{C}$

There was no significant difference in the amount of phenol from flue-cured and burley tobaccos when pyrolyzed in air at  $315^{\circ}\text{C}$  or at  $777^{\circ}\text{C}$ . In a nitrogen atmosphere at  $315^{\circ}\text{C}$  the difference in phenol between flue-cured and burley was in the same ratio as the difference in the smokes of the respective tobaccos (1.6 to 1).

A sample of flue-cured tobacco was extracted with hexane and then with 75% ethanol. The ethanol extract was chromatographed on a Celite column. The column was washed with methanol, acetone, ether, and hexane, respectively. I did not get the final figures on the amounts of phenol, but the greater the polarity of the solvent, the greater the yield of phenol. It was stated that the phenol yield was due partially to carbohydrates.

A four gram sample of flue-cured tobacco was extracted with 75% ethanol. To the ethanol extract  $5.0 \times 10^{-5}$  curie of C<sup>14</sup>-labeled glucose was added. The ethanol was evaporated and the sample was lyophilized. Four cigarettes were prepared and smoked. By radio assay this gave  $1.93 \times 10^{-7}$  counts/min. for phenol for the four cigarettes. It was stated that the uniformly labeled C<sup>14</sup> glucose contributed 41% to the total yield of phenol in sidestream and mainstream smoke.

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It was mentioned that the results for phenol may be higher than normal due to air oxidation, pyrolysis of lignins, pyrolysis of oxygenated compounds, and to carbon exchange. Also, flue-cured tobacco may have a catalytic effect on the formation of phenol.